ARTICLE 07 NIN COUPLING VALUES IN N=2 AND OXYGEN ELECTRONIC DENSITY Javier Silvestre (eeatom.blogspot com)

ABSTRACT

P34 NIN III: ns electron as origin of lobes in same n by curves coupling [6] is used to obtain z, $C_{POTI-AL}$ and C_{PEP} in n=2. These values are used in later studies and are applied here to estimate maximum Oxygen electron density with simple method. Estimate must corroborate Fluorine example that is in agreement with references [6].

By this method, Probability (P_i) calculations are directed to delimited r_i (Electronic extremes-nucleus radial distance) differentials rather than divisions (d). Thanks to this change, P_i curves of different electrons can be added or calculation centred on concrete r_i can be made.

KEYWORDS

NIN coupling, Electron Probability, Origin Electronic System (OES), Born Electronic System (BES), Victoria Equation.

INTRODUCTION

This is 7^{th} article of 24 dedicated to atomic model based on Victoria equation (Articles index is at end). A extern electronic extreme (EE_A) is indicated with a suffix (r_A, H_A or c_A), B intern with b suffix (r_B, h_B or c_B) and i suffix is used to both electronic extremes (EE_i). All abbreviations are compiled, in conjunction with those included in [6], at article end.

Electron with two EE has been introduced by Victoria Equation [1] and has been developed its geometry and probability [2-6] until achieving geometric and probabilistic coupling according to P34 NIN III [6]. This coupling between electron lobes (or Electronic Systems) by NIN rules allows extern electrons to be positioned by ns origin and provides approximate maximum electron density in n as P_i maximum contributed by the outermost Electronic System in n.

If in [6] maximum P_i is approximated by visual method from Pi vs. ri curve or from data with which figures have been made, curves overlap by P34 NIN III and maximum electron density are now studied in more detail using delimited r_i differentials. Initially, this study is centred on Oxygen lobes in n=2 to be later amplified to rest of atoms and lobes.

z, C_{PEP} and $C_{POTI-AL}$ (P32 C_{POTI} angular limit [5]) are calculated according [6] and summarized in P34 NIN III.

Born z by z coupling

Born Electronic System z (BES z or z_B) is provided by "P41 Electronic Charge (z) Coupling" [6] (1). Where BES is non-origin lobe and origin lobe is only ns electron external lobe. OES z or z_O is Origin Electronic System z.

(1)
$$z_{\rm B} = z_{\rm O}(\frac{(E_{\rm o})_{\rm B}}{(E_{\rm o})_{\rm O}})$$

(1) relates to ns origin electronic system (OES) because is the first in n quantum number and its z is known (P14 Effective nuclear charge in ns electrons [1]) and on which the rest are grouped. Anyway, all formulas that indicate O (Origin) and B (Born) can be transformed by considering born lobes (X and Y) that are located on the same n (2)

(2)
$$z(Y) = z(X) \frac{(E_o)_Y}{(E_o)_X}$$

P14 Effective nuclear charge in ns electrons, which subtracts one charge for each extern electronic system as loses energy, is only a good approximation when z and energy relations are in concordance (3). Where z_B^* is z_B , but applying P14 to system not OES.

$$(3) \frac{z_{o}}{z_{B}^{*}} \approx \frac{IE_{o}}{IE_{B}}$$

P14 is correct with ns external lobe and a good estimate when is applied on ns^2 external lobe. Applying P14, ns^2 has one unit less charge that ns since ns^2 is next in energy after ns (**Table 1**).

Table 1 - z values for ns and ns ² systems in n=2 applying P14											
Symbol	Li	Be	В	С	Ν	0	F	Ne	Na	Mg	Al
ns	1	2	3	4	5	6	7	8	9	10	11
ns ²		1	2	3	4	5	6	7	8	9	10

Considering (3) and accepting P14 for ns², Ionization Energy (IE) (experimental data in [7]) and Charge (z) ratios between ns and ns² electronic system are represented in **Figures 1 and 2** for n=2 and n=3 respectively. In both n quantum numbers, there is good overlap between two relationships. This fact implies that applying P14 to estimate ns² external lobe charge is a good approximation and can be corroborated with **Table 2** where z has been obtained by P41 (1). However, if this is done on 2p lobe where an additional unit of charge must be subtracted according to P14, **Figure 3** is obtained with a bad overlap between two ratios which is checked in Table 2. Charge correct values are in Table 2 for all electronic systems (lobes) located on n=2 of atoms with 2s electron having z = [1-8].







Table 2 – nuclear charge (z) value for Electronic Systems in n=2										
S	z 2s	z 2s ²	z 2p	z 2p ²	z 2p ³	z 2p ⁴	z 2p ⁵	z 2p ⁶		
Li	1									
Be	2	1,023845								
В	3	1,989542	0,655687							
C	4	2,970084	1,512369	0,698383						
N	5	3,957166	2,423395	1,511963	0,74237					
0	6	4,947863	3,362907	2,386446	1,52569	0,59158				
F	7	5,940713	4,318575	3,295186	2,370342	1,321885	0,658577			
Ne	8	6,93513	5,284351	4,224128	3,251903	2,122095	1,370589	0,721533		

CPOTI-AL Coupling

Probabilistic Orbital Tide Coefficient (C_{POTI}) is introduced in P30 Third Feliz Solution [5]. C_{POTI} can reach up to C_{POTI} Maximum Geometric Angular Limit or C_{POTI} Angular Limit ($C_{POTI-AL}$) when nucleus-orbit-angle (α_{NOA}) is 180 degrees and can not be overcome (P32) except by $C_{POTI-AL-d\to\infty}$ hypothesis [5]). $C_{POTI-AL}$ by division with C_{POTI} minimum [5] is employed (4):

(4) Cpotiminum =
$$\frac{\sqrt{2m_efz}}{\hbar} r_i^{1/2} C_{MON}$$

 C_{POTI} minimum is located in B intern electronic extreme by division (d) inclusion that provide C_{MON} and r_i values. 2s Nitrogen in its outermost lobe (n=2) has been taken by way of example. Division differences of 1 and 0.05 are chosen to observer consequent difference in minimum C_{POTI} obtained in (4) ($C_{POTI-AL}$). P14 can be used because 2s Nitrogen is origin lobe and therefore z=7-2=5 (Table 2). MON=10 according to P37.C. [6]. Search for C_{POTI} minimum can be performed considering this information and experimental IE [7]. Data are summarized in **Table 3**.

Table 3 - 2s Nitrogen lobe in $n=2$: $C_{POTI-AL}$ obtained usingdifferent division differentials							
d differentials	d with H→0	Cpoti-al					
1	20	3,6156985					
0,05	19,55	3,6156386					

Difference between d with H \rightarrow 0 is appreciable (20 and 19,55), although implies an effect on limited C_{POTI-AL} (difference $\approx 6*10^{-5}$). This difference in C_{POTI-AL} estimation is

even lower if d is higher since d increase implies smaller magnitude differences between divisions.

 $C_{POTI-AL}$ for lobes in n=2 from Li to Ne are in Table 4. 2s in n=2 (OES) is obtained by method of $C_{POTI-AL}$ by division with C_{POTI} minimum and rest of Electronic Systems in n=2 (BES) is approximated with (5). (5) is given by P43 C_{POTI} coupling [6].

(5)
$$C_{\text{POTI-B}} = C_{\text{POTI-O}} \sqrt{\frac{(E_{\circ})_{B}}{(E_{\circ})_{O}}}$$

Table	Table 4 – C _{POTI-AL} for Electronic Systems in n=2									
		Сь	РОТІ							
S	2s	$2s^2$	2р	2 p ²						
Li	3,120030815									
Be	3,359105728	2,403398153								
В	3,478217809	2,832516633	1,626856285							
С	3,560848848	3,068362468	2,189478264	1,487884432						
N	3,615638538	3,216562445	2,517271328	1,988249084						
0	3,654576548	3,318709246	2,736010032	2,304813508						
F	3,683620441	3,393507828	2,893245045	2,526847767						
Ne	3,706032043	3,450601332	3,011984264	2,692571622						
S	2 p ³	2 p ⁴	2p ⁵	2p ⁶						
Ν	1,393189102									
0	1,842764379	1,147537460								
F	2,143550200	1,600750723	1,129874022							
Ne	2,361971852	1,909133042	1,533973097	1,112989544						

Table 5 – $C_{POTI-AL}$ division for 2s OES (n=2)									
	Li	Be	В	С	Ν	0	F	Ne	
d	38,50	22,32	19,07	19,34	19,53	19,67	19,78	19,86	
MON	25	12,5	10	10	10	10	10	10	

Divisions, with accuracy = 0.01, that hold OES $C_{POTI-AL}$ are in **Table 5**. MON (P37 [6]) are also included in this Table 6. If MON is equal, divisions for $C_{POTI-AL}$ are similar and with a slight increasing trend with Atomic number. This MON influence in division that

has $C_{POTI-AL}$ evidences MON importance in morphology of geometric and probabilistic curves and therefore in $C_{POTI-AL}$.

MON Coupling

OES MON is supplied by "P37 OES MON" and BES MON is provided by "P39 MON Coupling" [6] (6). MON for lobes in n=2 from Li to Ne are in **Table 6**.

(6) MON_B = MON_o
$$\frac{(E_o)_o}{(E_o)_B}$$

Table	Table 6 – MON for Electronic Systems in n=2										
S	2s	2s ²	2p	2 p ²	2 p ³	2 p ⁴	2 p ⁵	2p ⁶			
Li	25										
Be	12,5	24,41776									
В	10	15,07885	45,75357								
С	10	13,46763	26,44857	57,27513							
Ν	10	12,6353	20,63221	33,06959	67,3519						
0	10	12,12645	17,84171	25,14199	39,32646	101,4234					
F	10	11,7831	16,20905	21,24311	29,53161	52,95468	106,2898				
Ne	10	11,53547	15,13904	18,93882	24,60098	37,69859	58,36905	110,875			

CPEP Coupling

BES C_{PEP} is given by (7) according to "P42 C_{PEP} as adapted Probability between a electrons pair". 2s OES C_{PEP} is taken equal to 1 because BES are born lobes whose Probability (Pi) are compared to OES. C_{PEP} is in **Table 7** for lobes in n=2 from Li to Ne.

(7)
$$C_{\text{PEP(B to O)}} = \sqrt{\frac{(E_{o})_{O}}{(E_{o})_{B}}}$$
 For $P_{B \text{ to O}}$ (PBORN TO ORIGIN)

Table	Table 7 – CPEP for Electronic Systems in n=2										
S	2s	2s ²	2p	2 p ²	2 p ³	2p ⁴	2 p ⁵	2p ⁶			
Li	1										
Be	1	1,397648									
В	1	1,22796	2,139008								
С	1	1,160501	1,626302	2,393222							

Ν	1	1,124069	1,436392	1,818505	2,595224			
0	1	1,101201	1,335729	1,585623	1,98309	3,184704		
F	1	1,0855	1,273148	1,457502	1,718476	2,301188	3,260212	
Ne	1	1,074033	1,230408	1,376184	1,56847	1,941612	2,415969	3,32979

H_i vs P_i representation with $C_{PEP}=1$

 H_i is circular orbital height. P_i and EE orbital circumference (c_i) are closely related through Compaction Factor (CF) [3-6]. Thus, H_i vs P_i is an approximation to H_i vs c_i and, consequently, provides an orbital geometry idea in two dimensions (height and width). Turn with radius= c_i allows to reach 3 dimensions. H_i vs P_i and not P_i vs H_i is for this reason of indirect geometric representation.

In **Figure 4 and 5** are A and B electronic extremes that correspond to electron in Oxygen that is in each one of six electronic systems that Oxygen have in n=2. In all lobes $C_{PEP}=1$, i.e. no C_{PEP} coupling, to observe initial positions before being referred to OES. Consequently, P34 NIN III is only with Geometric NIN Coupling (GNC) [6]. Figure 5 differs from 4 in that Y axis is enlarged from 0.3 to 1 A to achieve a broader view of the curve shape.





From both figures can be highlighted:

1) Electronic systems with higher IE present curves with P_i lower. Even considering that BES z are not integer (P41 [6]), order in P_i is deductible for their energies. Thus, curves located from lowest to highest probability are:

$$2s < 2s^2 < 2p < 2p^2 < 2p^3 < 2p^4$$

2) Curves shape is very similar although curves width differs. Role for Probabilistic NIN Coupling (PNC) is assumed by C_{PEP} (P34 NIN III [6])

3) In addition to similar curves shape, there are two geometric points that allow to imagine PNC:

3.1) Curves are linked at low d_B (where B subscript refers to B intern electronic extreme) See in Figure 4.

3.2) Division infinite points in H_i vs P_i representation are aligned with identical H_i fulfilling division infinite coupling between lobes (electronic systems) located in same n. In **Figure 6**, this H_i can be located above 7,55 $\cdot 10^{-12}$ m and can be specified with numerical treatment around 7,561 $\cdot 10^{-12}$ m.



P_i vs. r_i representation with C_{PEP}=1

Unlike the previous point, P_i is in Y axis since is r_i function. Also, is classic location in bibliography. Lobes are adjusted with GNC (**Figure 7** with $C_{PEP}=1$) as has been done in previous point with H_i vs. P_i . PNC view is represented later. P_i maximum varies slightly from 2s OES to the outermost $2p^4$ BES which is located at \approx 46 pm and agrees with 46 pm [8] and 44 pm [9]. Fluorine [6] and Oxygen have same 2s OES MON=10 (P37 [6]) and their P_i maximum for n quantum number where this outermost BES is located in a first approximation because:

1) $2p^4$ Outermost BES has a much higher probability than internal lobes as 2s OES. Specifically, in Oxygen case is on order of 3 times higher provided is assumed that global probability is referred to C_{PEP}=1. This model with GNC is compared in the following article with probability calculation when PNC has been produced.

2) Usually, there are more external electrons than internal electrons. In this case, there are 4 in 2p and 2 in 2s.

3) Curves and maxima are similar and therefore, differences between models are reduced.



Calculation method with r_i defined - Application to Probability

(8) subsequent use is indicated in [1]. (8) permits to know division associated with r_A and therefore r_A specific region can be studied.

(8) d =
$$\frac{E_{o}\lambda + \frac{F\lambda}{2r_{A}}}{F + E_{o}r_{A}}$$

1) Lobe Individual P_i (C_{PEP}=1)

For n=2, $2s^2$ and $2p^4$ Probability is in **Figure 8**. Figure 8 is bounded between 35 and 52 pm with r_i =0,5 pm variations. Maxima of both lobes are very close. This fact can be corroborated by **Figure 9** and **10** and corresponding **Table 8** (**Annex**) where maxima have been highlighted. P_i vs. r_i representations for $2s^2$ and $2p^4$ are in Figure 9 and 10 respectively.

2) Lobes P_i Sum (C_{PEP}=1)

Following steps are in this model:

2.1) Lobes that exist in a concrete n.

2.2) P_i vs. r_i curves for each lobe. All curves with C_{PEP}=1

2.3) Multiply P_i by electrons number that have that lobe; i.e. consider its electronic configuration (Oxygen n=2 shell has 2 electrons with lobe $2s^2$ and 4 electrons with lobe $2p^4$).

2.4) Lobes P_i summation. In Oxygen n=2 shell case, lobes P_i summation is represented in **Figure 11**. Resulting curve is similar to individual ones and has no discontinuities. P_i maximum is located at ≈ 46 pm and is also in agreement with 46 pm [8] and 44 pm [9].



 P_i vs. r_i curves can be constructed with lower r_i differentials to have a greater precision. Lobes P_i sum with C_{PEP} coupling (PNC) can be studied although resulting curve and P_i Maximum have little variation with what is seen at this point. Variations are somewhat greater when n quantum number increases, implying that MON decreases (P37 [6]) and P_i vs. r_i curves are diverted to higher r_i . These points are expanded in following article.

Pi representations with CPEP Coupling (Probabilistic Nin Coupling or PNC)

Above curves are transformed into PNC by C_{PEP} coupling. Data for C_{PEP} Coupling in oxygen n=2 shell are in **Table 7**. P_i vs. r_i representation with PNC for its six electronic systems is in **Figure 12**. All electronic systems are overlapped in infinite division and in wide range of B intern electronic extreme. With respect to A extern electronic extreme, curves overlap is performed up to near P_i maxima zone, from where distancing between P_i curves begins to become more noticeable as lobes are more energetically distanced (**Figure 13**).

 H_i vs. P_i representation is in **Figure 14**. $C_{POTI-AL}$ Coupling has been obtained from Table 4. Electronic extremes births junction is $H_i \approx 7,5$ pm as discussed previously. If instead of working with $C_{POTI-AL}$ and its $\alpha_{NOA}=180$ degrees, lower OES $C_{POTI-GAL}$ is selected, PNC is maintained.





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Abbreviations List

Suffix indicates electronic extreme considered and i suffix is used to both electronic extremes (EE_i). Following Table indicates abbreviations used in this theory and its use in article in question is marked with X. 7 is present article. Jump from "Article 09" to "Article 20" is consequence of second part inclusion.

Abbreviations Table										
Abbreviation	6	7	8	9	20	Meaning				
$\alpha_{ m NOA}$		Х				Nucleus-Orbit-Angle				
ao						Bohr radius				
AL						Angular Limit				
BES	Х	Х	Х	Χ		Born Electronic System				
ci	Х	Х	Х	Χ		EE Orbital circumference				
$C_{\rm F}$	Х		Х	Χ		Wavelength compaction factor				
C _{MON}	Х	Х				C _F without C _{POTI}				
C_{PEP}	Х	Х	Х	Χ		Probability electrons pair coefficient				
C _{POTI}	Х	Х	Х	Χ		Probabilistic Orbital Tide in Third Feliz Solution				
C _{POTI-AL}		Х	Х	Χ		C _{POTI} Angular Limit				
C _{POTI-GAL}			Х			CPOTI Geometric Angular Limit				
C _{POTI-LAG}			Х			C _{POTI} Lobe always growing				
d	Х	Х	Х	Χ		Birth wavelength division or simply, division				
EE	Х	Х	Х	Χ		Electronic extreme				
Eo	Х	Х	Х	Χ		Initial, birth or output energy				
Ei			Х			EE energy				
Eki						EE kinetic energy				
EPi						EE potential energy				

ES					Equi-energetic state
f	Х				Constant in Victoria Equation
F		Х			Constant f multiplied by z
GAL					Geometric Angular Limit
GNC	Х	Х	Χ	X	Geometric NIN Coupling
h					Planck's constant
ħ	Χ		Χ		Reduced Planck's constant
hi					Planck's constant adapted to EE
H _i	Х	Χ	Χ	Χ	EE Circular orbit height
IE	Χ	Χ	Χ	X	Ionization Energy
m _e			Χ		Electron mass
mi					EE mass
J	Х				C _F order in Second Feliz Solution (From x=1 to J)
K _P					Probability constant in Variable C _F
$\lambda_{Birth} \lambda$		Χ	Χ		Birth wavelength
$\lambda_{ m c}$					Electron classic wavelength
λ_i					EE wavelength
$\lambda_{i-Birth}$					EE wavelength when $d \rightarrow \infty$
М	Χ				MON (Modified Orbital Number)
MON	Х	Χ	Χ	Χ	Modified Orbital Number
NIN	Χ	Χ	Χ	X	Negative in Negative (Electron in electron concept)
OAM					Orbital Angular Momentum
OES	Х	Х	Χ	X	Origin Electronic System
OPA			Χ		Orbital Planes Axis
Pi	Χ	Χ	Χ	X	EE Probability
Р	Χ				PEP (Principal Electronic Part)
PEP	Χ				Principal Electronic Part
PNC	Х	Х	Х	Χ	Probabilistic NIN Coupling
P _{Y to X}	Х				P _y with respect to X lobe
ri	Х	Х	Х	Χ	Distance between nucleus and EE
Vi			Χ		EE velocity
Z	Χ	Χ	Χ	X	Effective nuclear charge
Z		Χ	Χ		Atomic number

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Annex

Table 8 - Oxygen. EEA Probability (PA) – Maximum PA zone for 2s ² and 2p ⁴ with CPEP=1								
	ci-prob	abilidad						
ri	2s2	2p4						
3,5E-11	5,2558E-18	1,5206E-17						
3,55E-11	5,3026E-18	1,5342E-17						
3,6E-11	5,3462E-18	1,5470E-17						
3,65E-11	5,3866E-18	1,5589E-17						
3,7E-11	5,4241E-18	1,5700E-17						
3,75E-11	5,4585E-18	1,5802E-17						
3,8E-11	5,4902E-18	1,5898E-17						
3,85E-11	5,5190E-18	1,5985E-17						
3,9E-11	5,5450E-18	1,6066E-17						
3,95E-11	5,5685E-18	1,6140E-17						
4E-11	5,5893E-18	1,6207E-17						
4,05E-11	5,6076E-18	1,6268E-17						
4,1E-11	5,6234E-18	1,6323E-17						
4,15E-11	5,6368E-18	1,6372E-17						
4,2E-11	5,6478E-18	1,6415E-17						
4,25E-11	5,6565E-18	1,6453E-17						
4,3E-11	5,6630E-18	1,6485E-17						
4,35E-11	5,6673E-18	1,6512E-17						
4,4E-11	5,6695E-18	1,6535E-17						
4,45E-11	5,6696E-18	1,6552E-17						
4,5E-11	5,6677E-18	1,6565E-17						
4,55E-11	5,6638E-18	1,6574E-17						
4,6E-11	5,6579E-18	1,6579E-17						
4,65E-11	5,6502E-18	1,6579E-17						
4,7E-11	5,6407E-18	1,6576E-17						
4,75E-11	5,6294E-18	1,6568E-17						
4,8E-11	5,6164E-18	1,6558E-17						
4,85E-11	5,6017E-18	1,6543E-17						
4,9E-11	5,5853E-18	1,6526E-17						
4,95E-11	5,5674E-18	1,6505E-17						
5E-11	5,5480E-18	1,6481E-17						
5,05E-11	5,5271E-18	1,6455E-17						
5,1E-11	5,5048E-18	1,6425E-17						
5,15E-11	5,4811E-18	1,6393E-17						
5,2E-11	5,4560E-18	1,6359E-17						